3. *Maximum Likelihood Cosine Inversion for Dynamic Range Extension of Interferometric Spectra*

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Objective: To demonstrate the utility of optical interferometry in the UV and visible spectral regions for precise and accurate optical isotope ratio determinations; and to characterize "Maximum Likelihood Inversion" as an approach for obtaining spectra with physically meaningful noise distributions.

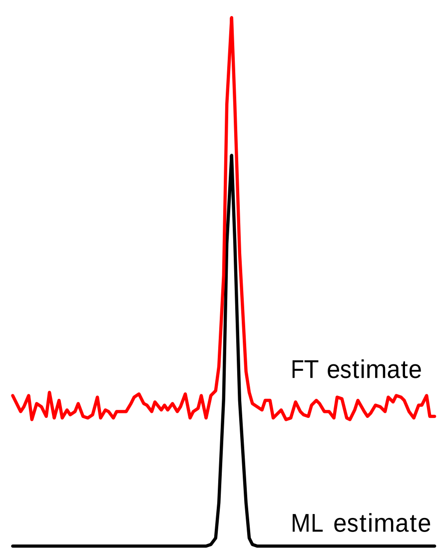
Problem: Fourier transform spectrometry has dominated grating spectrometry in the infrared spectral region for some years, due to the so-called multiplex advantage associated with acquiring data simultaneously at all available wavelengths. Technical advances in computing technology, control systems, and optical component fabrication over the past decade have made possible the successful operation of Michelson interferometers at shorter wavelengths – extending well into the UV – but without the multiplex advantage shown in the IR. Indeed, FT/UV is widely characterized as having a "multiplex disadvantage" resulting from the artificial redistribution of noise in the spectrum by the mathematical Fourier transform used to derive a spectrum from a Michelson-measured interferogram.

Approach: A recent study shows the promise of an alternative method for deriving the spectrum from an interferogram, distributing the noise at the frequencies where it belongs. By employing "Maximum Likelihood Inversion" [Bialkowski, Appl. Spectrosc. 52, 591 (1998)], we are working to achieve adequate accuracy and dynamic range for practical optical isotope ratio measurement. This program pivots on the implementation of an expectation-maximization (EM) implementation of Maximum Likelihood (ML) Inversion, enabling dynamic range enhancement of line emission spectra. The published algorithm has been implemented and tested with small data segments on a desktop computer. The algorithm, particularly scalable to multiple processors, has been ported to a parallel architecture. Preliminary experiments have been performed to validate the parallelization. Because the computation of this inversion is costly, several strategies have been identified to effectively scale the approach to complete data sets.

Results and Future Plans: Scalability studies indicated excellent performance for the parallel implementation of the algorithm, with minimal loss in performance from inter-processor communication. The parallel implementation is portable between parallel computers, using standard libraries. Convergence performance was poor, and precluded inversions of even moderate resolution spectra.
Three technical approaches have been identified to achieve practical transform times with this iterative algorithm:

- region-of-interest identification and fitting
- filtered initial parameter estimation
- application of an accelerated EM algorithm.

Collaboration with scientists in the High-performance Computing and Statistical Engineering divisions has and will continue to be of utmost importance for further progress.



Maximum likelihood and Fourier transform estimate.